PSI SciDAC: Dynamic Code-Coupling Roadmap

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**Plasma-Material Interaction SciDAC
Dynamic Code Coupling Working Group
August 12, 2020**

Objective: Develop fundamental understanding of the dynamics of the recycling of main ion species

Three different high Priority Research Objectives (PRO) have been identified that can be experimentally validated

1. Physics of the ELM Density Cycle
- High impact, clear example of coupled wall/plasma physics
- Goes beyond previous studies by including predictive W-wall model
  - Pigarov et al POP 2014, Krashenninikov et al PPCF 2015, Smirnov et al POP 2020

2. Recycling Physics Including Multiple Species
- Understand atomic D vs molecular D2 recycling physics
- Understand the impact of He implantation on H recycling in W
  - Bykov et al Physica Scripta 2020, upcoming DIII-D experimental campaign

3. Impact of Recycling on Divertor Turbulence
- Determine modes of instability and dominant damping mechanisms
- Impact on saturated amplitude of turbulence and turbulent transport
  - Krashenninikov et al POP 2006

PRO 1: Pedestal particle refueling during the ELM cycle

Physics: For large ELMs, the pedestal refueling time is controlled by outgassing from the wall [Pigarov POP 2014, Krash PPCF 2015]

- If the number of particles expelled by the ELMs is larger than the steady-state number of particles stored in the SOL + divertor, then a significant fraction will be stored in the wall and then released on the wall outgassing timescale

Goal: Determine the critical ratio $\eta = \Delta N_{ped}/N_{SOL+div}$ **for different scenarios**

- Previous work focused on C walls
- Here, we want to extend understanding to W PFCs
- Phenomenological 1D and 2D model should be sufficient for qualitative understanding

Issues: Need to tune phenomenological parameters to experimental observations

- Spatial distribution and energy distribution of traps
- Initial distribution of H? Would like this to correspond to a dynamic steady-state, including ELMs, but may also need to simulate prehistory for certain scenarios
- Need to sweep strike point to emulate the way that the magnetic perturbations caused by ELMs modify the strike point location

PRO 1: Pedestal particle refueling during the ELM cycle

Strategy:

- Complete development of UEDGE/FACE simulation capabilities in FY21 using IPS
- Complete dynamic 2-way SOLPS/Xolotl workflow in FY21 using IPS
- Explore physics of the coupled models from FY21 through FY22
- Develop collaborations with W-walled tokamak facilities to enable validation studies
  - JET, EAST, WEST are all good candidates

HPC Tools:

- **Plasma:** UEDGE (fluid neutrals) and SOLPS (kinetic neutrals and molecular species)
- **Wall:** FACE (H only) and Xolotl (both H and He, e.g. useful for ITER startup)
- **Coupling Framework:** IPS believed to be sufficient at this time

Team:

- **Point of Contact:** Roman
- **Team Members:** Sergei, Roman, Maxim, Ilon, Jerome, Ane Lasa, John, Jeremey
- **UEDGE/FACE:** Roman, Maxim
- **SOLPS/Xolotl:** Ane Lasa, John, Jeremy

Timeline for ELM density pedestal recovery with active wall

	FY 20	FY 21				FY 22			
	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
2D UEDGE/FACE coupling using IPS framework (Roman, Maxim)	High	High	High	Completed					
Testing, comparing with 1D results		High	Completed						
Investigation of response characteristics and impact of initial conditions		High	High	Completed					
Effects of traps and wall profiles on response times, saturation layer model (FACE)		High	High	Completed					
Impact of divertor plasma parameters on wall conditions (UEDGE/FACE)			High	Completed					
2D modeling of ELM and density pedestal recovery (Roman, Maxim)			High	High	High	High	Completed		
Studies of ELM size effects, comparison with experiment			High	High	High	High	Completed		
Detachment, separatrix sweeping effects			High	High	High	Completed			
Cross-benchmark with Xolotl				High	High	High	Completed		
2D SOLPS/Xolotl coupling using IPS framework (Ane Lasa, John, Jeremy, Roman, Maxim)		High	High	High	High	High	High	High	Completed
Implement & test SOLPS/Xolotl coupling -- build on UEDGE/FACE workflow		High	High	Completed					
Cross-benchmark with UEDGE/FACE				High	High	High	Completed		
Perform physics studies including impact of He in W						High	High	High	Completed

High priority task (dark green)   **Completed milestone** (light green)

Fusion Energy Sciences

PRO 2: Recycling Physics Including Multiple Species

Physics: Including multiple species, e.g. atoms, molecules, and He, can have an important impact on dynamic recycling

Goal: Compare simulated predictions of particle densities and fluxes to experimental measurements

- Compare recycled flux of D atoms to D_2 molecules
  - Bykov et al Physica Scripta 2020
- Understand changes due to biasing, ELMs, large pellets to edge/div/sol
- Understand changes due to prior He loading of W PFCs
  - Planned future DIII-D experimental campaign [Sinclair, et al]

Simplifying Assumptions

- Focus on short term recycling rather than long term recycling
- Ignore low-Z impurities, such as C, Be, etc.
- Do not track dynamic recycling of He itself

PRO 2: Recycling Physics Including Multiple Species

Strategy:

- Use MD (LAMMPS) simulations to develop a set of reduced parameters that describe H transport in the presence of He implanted within W PFCs [Brian, 2021]
- Explore the physics of reduced models for H transport using Xolotl and FACE with and without He [Ane Lasa, 2022]
  - Determine under which conditions He in W can have significant impact on H dynamic recycling from W using Xolotl [Ane, Brian, Jerome, 2022]
- Perform plasma-wall coupled simulations to understand the physics of dynamic recycling
  - Determine whether significant impact of He in W on H dynamic recycling may be expected in DIII-D experiments [Ane, Brian, Jerome, 2022]

HPC Tools:

- **Plasma:** SOLPS and UEDGE
- **Wall:** Xolotl or FACE
- **MD Modeling of Transport Coefficients:** LAMMPS
- **Coupling Framework:** At this point, we believe that IPS should be sufficient

Team:

- **Point of Contact:** Jerome
- **Team Members:** Ane Lasa, Brian, Jerome, Maxim, Roman
- **UEDGE/Xolotl:** Ane Lasa, Roman, Jerome

Dynamic recycling from W PFCs loaded with He

Tasks	FY20	FY 2021				FY 2022			
	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
LAMMPS & Xolotl simulations to examine effects of He in W on dynamic recycling vs pristine W									
• MD simulations of He effects on D transport in W. Next step is to use Xolotl to integrate MD simulations [Brian]	�								
• Physics analysis with Xolotl: explore wider range of parameters (He/H flux, temperature (Q), He energy distribution) for ELMs [Ane Lasa]									
Theoretical & computational analysis of dynamic H recycling from W with FACE & Xolotl with/without He									
• Characterization of wall response to plasma fluctuations and role of induced vs thermal desorption (D/D2)									
• Reduced 0D model (integro-differential equation?) to mimic fast wall response without/with He [Jerome]									
• Determine the conditions for He in W to have significant impact on H dynamic recycling [Jerome, Brian, Ane]									
Simulate dynamic recycling from W pre-exposed to He during and between ELMs with UEDGE + Xolotl/FACE									
• Determine whether significant impact of He in W on H dynamic recycling is expected for DIII-D experiments [All]									
• Coupling Xolotl to UEDGE through IPS [Ane Lasa, Roman]									
• OMFIT workflow to model ELMs and material response in DIII-D divertor with UEDGE+Xolotl [Jerome, Orso]									

Fusion Energy Sciences

PRO 3: Impact of Recycling on Turbulence

Physics: Edge turbulence can be modified by wall physics because it introduces new dissipation and feedback mechanisms

Goal: Understand which plasma-wall interactions play an important role in modifying linear growth rates and nonlinear turbulence saturation levels

Physics:

- Ionization and charge exchange collisions shown to have a direct impact [Umansky unpublished]
- Time delay between wall response to plasma fluxes may also have an impact
- **Key Feedback Process [Krash 2006]:** Radiation emitted by neutrals heats the wall, and leads to increased outgassing of neutrals

- Short time recycling determined by near-surface layers (w = 10 nm – 1 um)
  - Rough estimate of wall diffusion, $D \sim 10^{-8}$ m^2/s, implies freq's $D/w^2 \sim 10^4$-10^8 Hz,
  - Wall timescales should match plasma turbulence freq's 10^4-10^5 Hz

PRO 3: Impact of Recycling on Turbulence

Strategy:

- Would like to start with a **simple wall model** that can be directly implemented within BOUT++ and be used to control wall timescales
- Explore explicit coupling between BOUT++ and FACE using IPS
- If explicit coupling is too expensive, then implement and explore implicit coupling between BOUT++ and FACE

HPC Tools:

- **Plasma:** BOUT++
- **Wall:** Analytic model → FACE → Xolotl
- **Coupling Framework:** IPS is a good start, but may need to move towards in-memory coupling such as ADIOS, etc.

Team:

- **Point of Contact:** Maxim
- **Team Members:** Sergei, Roman, Maxim, Jerome, Ilon
- **Analytic model:** Sergei, Roman, Jerome
- **BOUT++/FACE:** Maxim, Roman

Timeline for modeling turbulence with active wall

	FY 2021				FY 2022			
	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
BOUT++/FACE explicit coupling using IPS framework (Roman, Maxim)	🟩	🟩	🟩					
Testing, comparing with previous BOUT++ results			🟩					
Modeling of wall outgassing impact on divertor instabilities, comparison with experimental data (Roman, Maxim)				🟩	🟩	🟩	🟩	🟩
Simulation of wall impact on linear instability growth rates, comparison with analytic theory				🟩	🟩	🟩	🟩	
Simulation of nonlinear instabilities, comparison with experimental data						🟩	🟩	🟩
Model extensions (Roman, Maxim)		🟩	🟩	🟩	🟩	🟩	🟩	🟩
Theoretical investigation of timescales/wall coupling		🟩	🟩	🟩	🟩			
Simplified 0D model development					🟩	🟩	🟩	
Implementation/ benchmarking of 0D model							🟩	🟩
Explore/implement implicit BOUT++/FACE coupling if necessary					🟧	🟧	🟧	🟧

🟩 **High priority task**   🟩 **Completed milestone**

Additional Material

Initialization:

- Plasma and wall are weakly coupled when recycling = 1, because the ratio of neutral species, e.g. ratio of D2 molecules to D atoms, is the only coupled part of the problem
  - Excellent approximation: solve for plasma, then solve for wall given Q_{plasma}, then iterate to determine self-consistent solution

Objective: Determine the erosion rate of material surfaces that are exposed to large transient events such as ELMs

- **Requires accurate models for many nonlinear processes**
  - Need to determine when kinetic effects are important

- **Plasma model**
  - Fluid models: SOLPS, UEDGE, BOUT++ exchange density, momentum, energy
  - Kinetic models: COGENT, hPIC

- **Sheath model**
  - Energy and angle distribution of incoming/outgoing fluxes

- **Surface model**
  - Reflection & sputtering yields
  - Implantation concentration and depth profile

- **Wall model**
  - Material evolution
  - Neutral outgassing flux
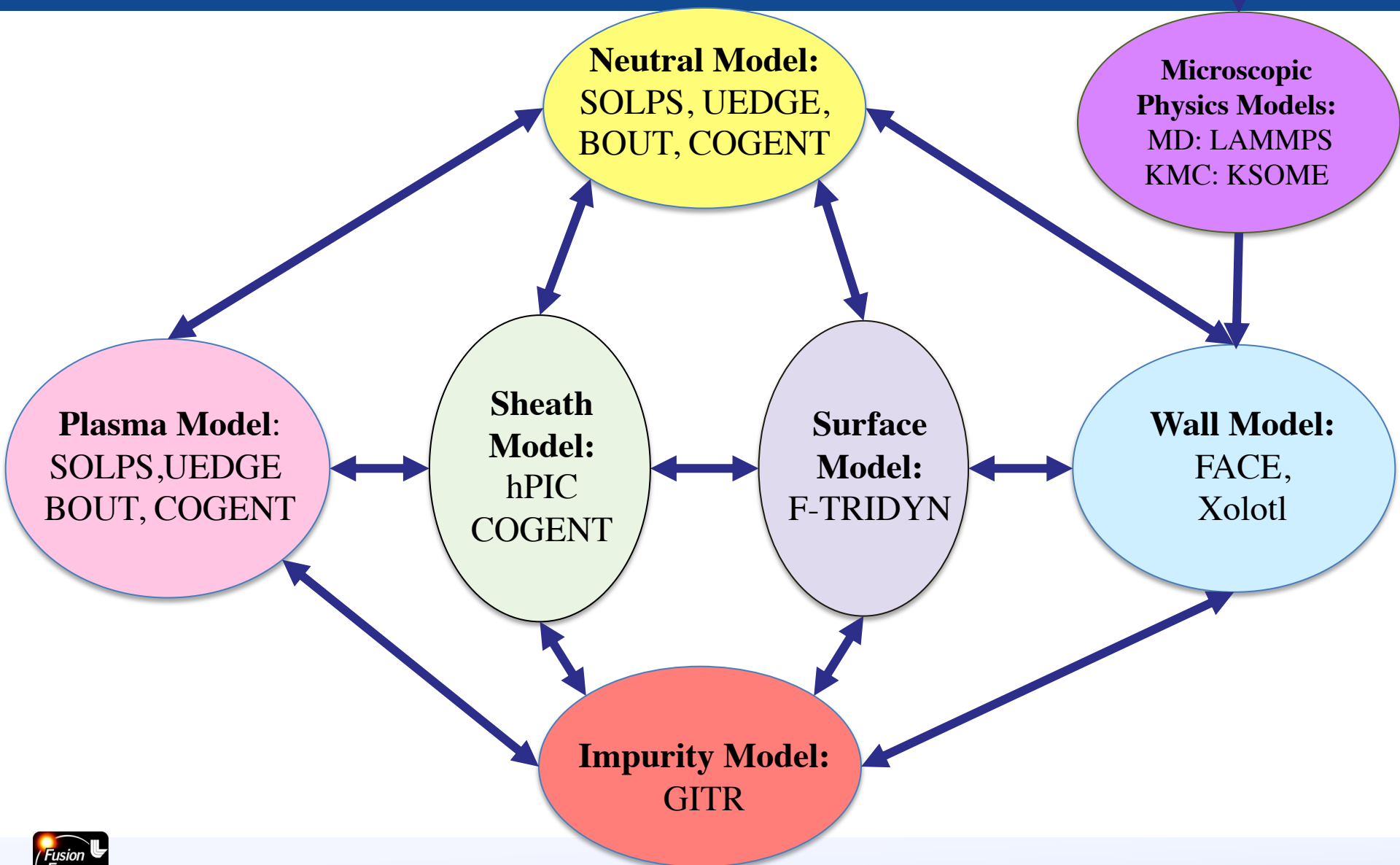
Objectives in the PSI SciDAC-4 proposal

- In this project, we will couple the **SOLPS** plasma transport and **BOUT++** plasma turbulence codes to **wall physics models** of varying sophistication, with the end-goal of coupling to the **Xolotl** multiscale materials modeling code.

- We will verify the models against predictions of analytic theory; e.g. by comparing linear dispersion relations of the modes in simplified geometry. Then we will **perform nonlinear** simulations that can be **compared to experiment** & used to **validate the wall models**.

- **Code coupling will first be developed using a file-sharing protocol**. However, it is anticipated that the dynamic coupling could be tight, in which case more advanced in-memory coupling and/or implicit coupling methods might be required.

- At the outcome of this project we will have two packages of coupled state-of-the-art plasma-wall codes: (i) **SOLPS/Xolotl** and (ii) **BOUT++/Xolotl** capable of simulating a wide range of synergistic plasma-wall effects including the:
  - ELM density cycle
  - Impact of hydrogen recycling on heat fluxes delivered to the divertor, and
  - Coupling of divertor turbulence to the wall absorption and desorption dynamics
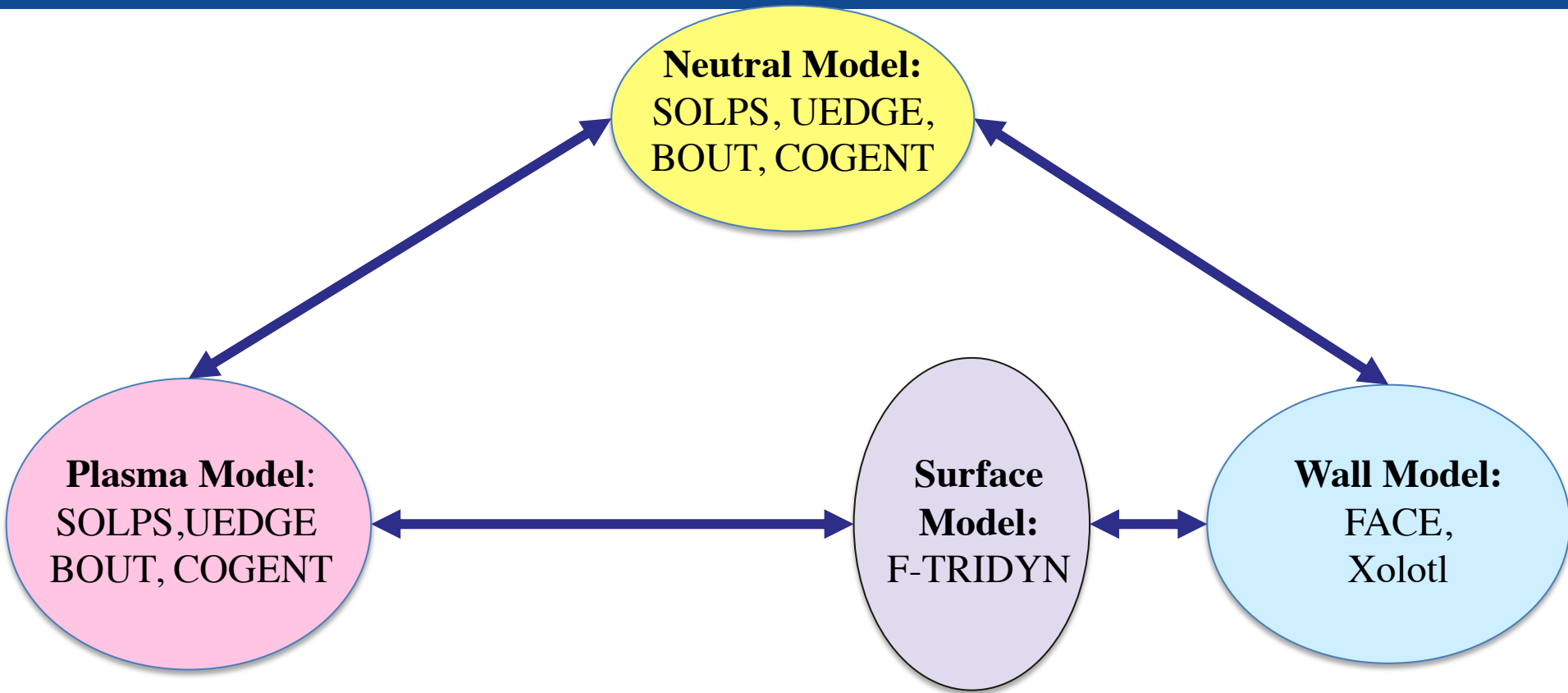
Coupling the Models: The final frontier.
To boldly go where no [one] has gone before!
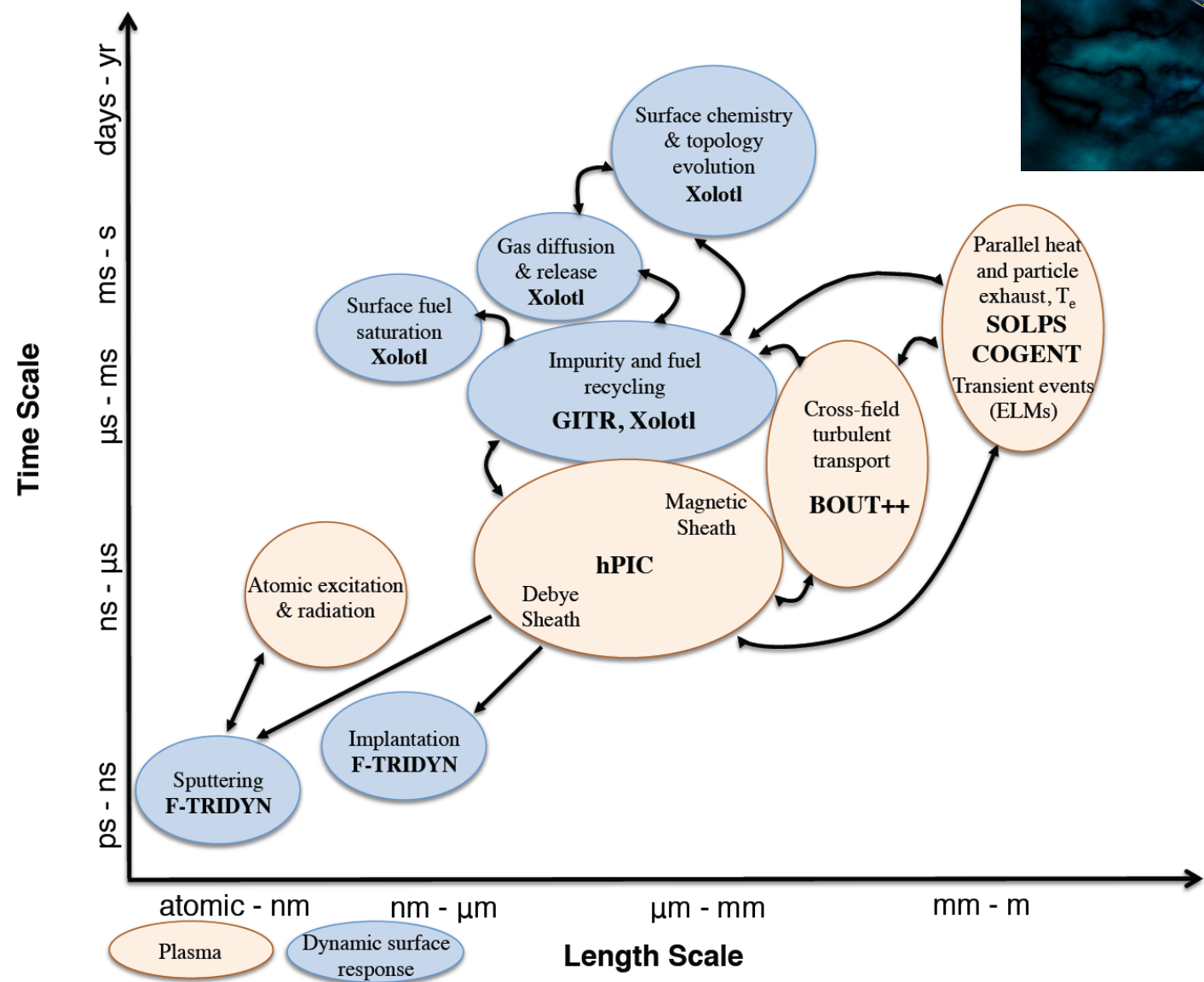
Coupled Plasma-Wall Hierarchy

Initial Target: simplified recycling flowchart

Plan for Simplified Main Ion Recycling

Wall-directed fluxes for all species → Energy-angle distribution of wall-directed species → Implantation profile of wall-directed species: particles and energy →

Plasma & Neutral Model: SOLPS, UEDGE, BOUT, COGENT → **Sheath Model: hPIC COGENT Analytic** → **Surface Model: F-Tridyn Analytic** → **Wall Model: FACE, Xolotl**

← Plasma-directed fluxes of charged species | ← Reflected & sputtered energy-angle distribution | ← Material composition

Plasma directed neutral fluxes

Even Simpler: focus on plasma-wall coupling alone

Wall-directed fluxes for all species

Energy-angle distribution of wall-directed species

Implantation profile of wall-directed species: particles and energy

Plasma & Neutral Model: SOLPS, UEDGE, BOUT, COGENT

Analytic

Wall Model: FACE, Xolotl

Plasma-directed fluxes of charged species

Reflection & sputtering coefficients

Plasma directed neutral fluxes
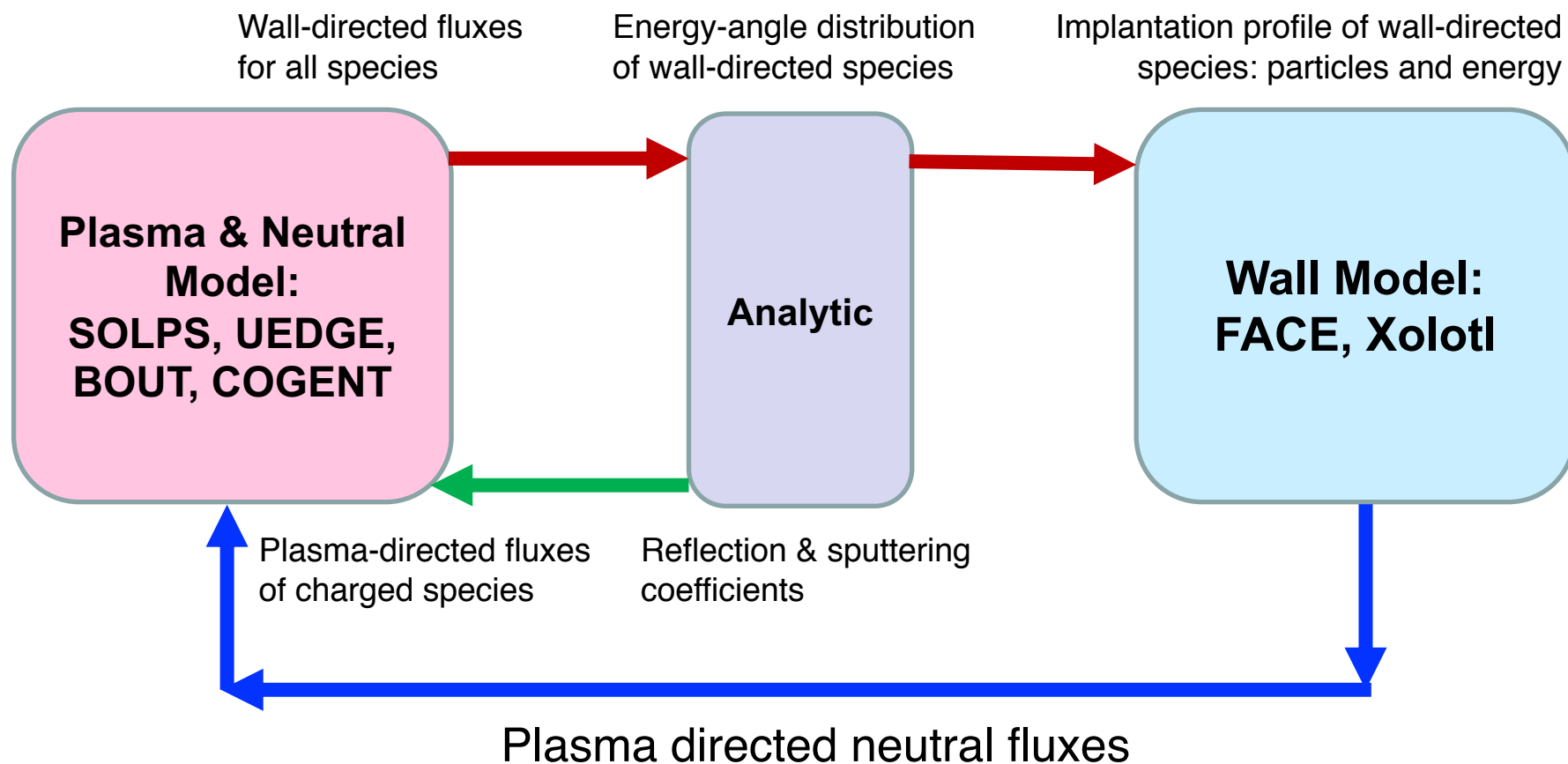
Example: UEDGE ⬅➡ FACE Coupling Scheme

- **File-based coupling sufficient**
- **Complexity: ~2 floats * species * wall locations * iterations**

BASIS or Python shell

$$\boxed{\textbf{UEDGE}}$$

Particle flux: Γ_{in}
Heat flux: Q_{in}

Recycling coefficient: $R = \Gamma_{out}/\Gamma_{in}$

Particle flux from wall: Γ_{out}

$$\boxed{\textbf{FACE}}$$

Coupling time step Δt:
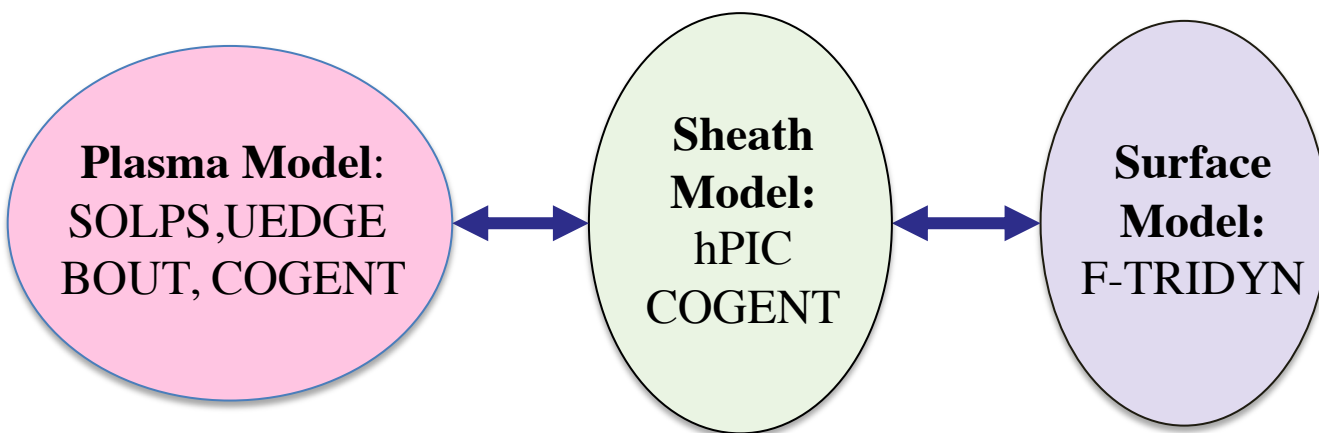**Both codes can sub-cycle with smaller**
step till convergence on Δt
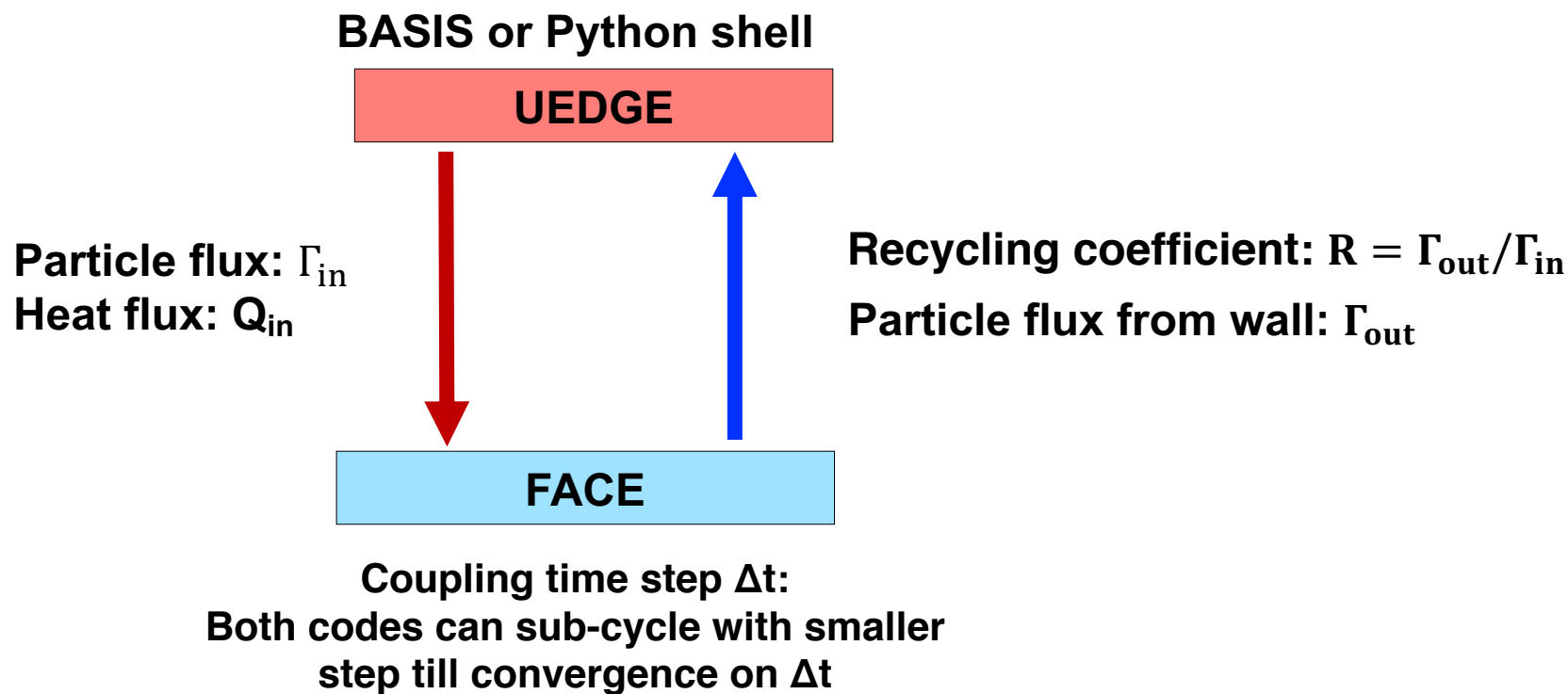
Implementation Needs: Dynamic Recycling

- ## SOLPS ←→ Xolotl

    - Implementation of Xolotl → SOLPS/EIRENE coupling
        - Neutral species fluxes → EIRENE input

    - Extension to IPS driver
        - Build upon tools developed for 2018 Theory Milestone
        - Explore convergence of coupling algorithms

    - Explore physics of wall coupling (time dep. vs. steady-state)

- ## Team (?): Ane, Sophie, Wael, John Canik, Jeremy Lore

Implementation Needs: Dynamic Recycling

- **UEDGE ←→ FACE … ←→ Xolotl**
  - BASIS
  - Python
  - **IPS**

- **BOUT++ ←→ FACE … ←→ Xolotl**
  - Python
  - **IPS**
  - ADIOS → CVODE/SUNDIALS

- **COGENT ←→ FACE … ←→ Xolotl**

- **Team:** Ane, Sophie, Wael, Maxim, Roman, Ilon, Debo

Initial Target: kinetic impurity erosion

Plasma Model: SOLPS, UEDGE BOUT, COGENT ↔ Sheath Model: hPIC COGENT ↔ Surface Model: F-TRIDYN

Implementation Needs: Impurity Erosion

- **UEDGE ←→ FACE … ←→ Xolotl**
  - BASIS
  - Python
  - **IPS**

- **BOUT++ ←→ FACE … ←→ Xolotl**
  - Python
  - **IPS**
  - ADIOS → CVODE/SUNDIALS

- **COGENT ←→ FACE … ←→ Xolotl**

- **Team:** Ane, Sophie, Wael, Maxim, Roman, Ilon, Debo

Implementation Needs: Thrust 3

- **COGENT ⟷ hPIC ⟷ F-Tridyn**
  - Python
  - **IPS**
  - ADIOS

- **Team:** Ilon, Debo, Davide, John Drobny

Thrust 3: Dynamic Coupling Timeline

2018	2019	2020	2021	2022

Dynamic Main Ion Recycling

UEDGE ←→ FACE (2019–2020)

UEDGE ←→ Xolotl (2020–2022)

SOLPS → Xolotl (2018–2020)

SOLPS ←→ Xolotl ? (2020–2022)

BOUT ←→ FACE (2021–2022)

BOUT ←→ Xolotl (2022)

Impurity Production & Recycling

COGENT → hPIC → F-TRIDYN (2020–2022)

COGENT ←→ hPIC (2022)